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NMR quantification in the verification of compounds: Simple to complex mixtures

Joshua M Hicks
Catalent Pharma Solutions, USA

Quantification is one of the most important pieces of information when using compounds in testing. It is important that the correct concentration is used when measuring within applications such as monitoring of reactions, proteinligand binding for the measurement of binding constants, dosage, fragment based screening, and monitoring of branching rates of polymers, among others. Such rate limiting steps are self evident in compound library screening where one must verify concentration in a high throughput means. With the improvements in software and NMR instrumentation, it is possible to have on the fly verification where concentration can be a key part of the verification process. Since the submitter has knowledge of the (suggested) structure, a known submission mass and a volume, the calculations for integral accounting and assignment can be output. Concentration is a key aspect because deviations are indicative of compounds purity from other compounds as well as impurities not directly observable by NMR such as salts. Additionally the solubility of the compound and stability are observed due to large changes in calculated versus measured concentration. All important aspects when validating a regular method for development/validation of definitive verification of a compound or mixture of compounds.

Biography

Joshua M Hicks has completed his PhD from Oregon State University in 2005 from the department of Biochemistry & Biophysics, and a Postdoctoral tenure at Stockholm University. He is a Lead Scientist in the Structural group at Catalent, a premier drug development, delivery and supply partner organization for drugs, biologics, and consumer health products. He has been highly active in the design, development and implementation of NMR applications in pharmaceutical applications for over 9 years.

joshua.hicks@catalent.com
josh.m.hicks@gmail.com

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